

Claims

1. A crystal of a RAD51-BRC repeat sequence complex.
2. A crystal according to claim 1 having the orthorhombic space group $P2_12_12_1$, and unit cell dimensions $a = 57.30 \text{ \AA} \pm 5\%$,
5 $b = 59.14 \text{ \AA} \pm 5\%$, $c = 77.20 \text{ \AA} \pm 5\%$.
3. A crystal according to claim 1 which diffracts X-rays for the determination of atomic coordinates of the complex to a resolution of better than 2.0 \AA .
4. A crystal according to claim 1 having the three
10 dimensional atomic coordinates of Table 1.
5. A RAD51-BRC repeat sequence chimaera protein in which the RAD51 is covalently joined to the BRC repeat sequence.
6. A RAD51 paralogue-BRC repeat sequence chimaera protein in which the RAD51 paralogue is covalently joined to the BRC
15 repeat sequence.
7. A nucleic acid encoding the chimaera protein of claim 5 or 6.
8. A mutant RAD51 which has been modified to reduce or eliminate the tendency of RAD51 to spontaneously aggregate
20 into high molecular weight complexes.
9. A mutant RAD51 which has been modified by substitution, deletion and/or addition of at least one amino acid in the 85-GFTTATE-91 sequence of human RAD51, or the corresponding sequence in other forms of RAD51.
- 25 10. A nucleic acid encoding the mutant RAD51 of claim 8 or 9.
11. Use of the mutant RAD51 of claim 8 or 9 in an assay for identifying compounds which interact with or form part of a RAD51 pathway.

12. A compound which is identified by the method of claim 11.

13. A method of homology modelling comprising the steps of:

(a) aligning a representation of an amino acid sequence of a target protein of unknown three-dimensional structure with the amino acid sequence of the RAD51 or the BRC repeat sequence of Table 1 to match homologous regions of the amino acid sequences;

(b) modelling the structure of the matched homologous regions of said target protein of unknown structure on the corresponding regions of the RAD51 or BRC repeat sequence structure as defined by Table 1; and

(c) determining a conformation for said target protein of unknown structure which substantially preserves the structure of said matched homologous regions.

14. A method for determining the structure of a protein, which method comprises;

providing the co-ordinates of Table 1, and

positioning the co-ordinates in the crystal unit cell of said protein so as to provide a structure for said protein.

15. A method for determining the structure of a compound bound to RAD51 or a BRC repeat sequence, said method comprising:

providing a crystal of a complex in which a compound is bound to RAD51 or a BRC repeat sequence; and

determining the structure of said complex by employing the data of Table 1.

16. A computer-based method for the analysis of the interaction of a molecular structure with RAD51 or BRC repeat sequence, which comprises:

providing the structure of RAD51 or a BRC repeat sequence as defined by Table 1;

providing a molecular structure to be fitted to said

RAD51 or BRC repeat sequence structure; and

fitting the molecular structure to the RAD51 or BRC repeat sequence structure.

17. A computer-based method for the analysis of the
5 interaction of a molecular structure with RAD51 or BRC repeat sequence, which comprises:

providing the coordinates of at least two atoms of RAD51 or a BRC repeat sequence structure as defined by Table 1;

10 providing a molecular structure to be fitted to said coordinates; and

fitting the structure to the said coordinates.

18. A method of determining the biological activity of a compound, which comprises:

15 identifying a compound which fits to RAD51 or a BRC repeat sequence by performing the method of claim 16 or 17;

obtaining or synthesizing the compound; and

testing the compound in an *in vivo* or *in vitro* biological system in order to determine the activity of the compound.

19. A compound which is identified by the method of claim 16
20 or 17.